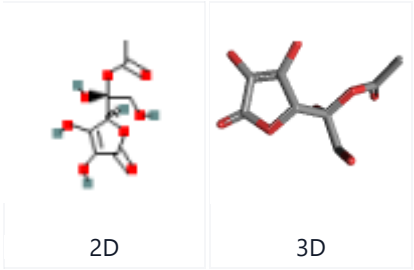
PubChem

COMPOUND

Vitamin c acetate

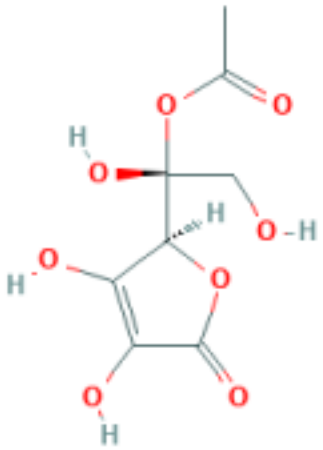
PubChem CID	129845507
Structure	 2D 3D
Molecular Formula	$C_8H_{10}O_8$
Synonyms	vitamin c acetate
Molecular Weight	234.16 g/mol *Computed by PubChem 2.1 (PubChem release 2021.05.07)*
Dates	Create: 2017-09-13 Modify: 2026-06-27

1 Structures

1.1 2D Structure

Structure Search Get Image Download Coordinates

Chemical Structure Depiction



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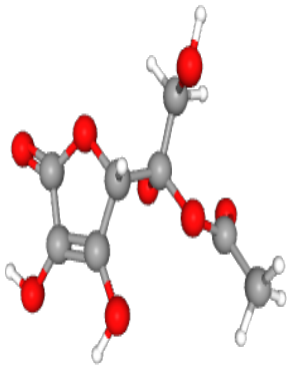
1.2 3D Conformer

Structure Search Get Image Download Coordinates

Interactive Chemical Structure Model

- (•) Ball and Stick
- ( ) Sticks
- ( ) Wire-Frame
- ( ) Space-Filling
- [x] Show Hydrogens
- [ ] Animate



First Previous Conformer 1 of 10 Next Last

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

[(1*R*)-1-[(2*S*)-3,4-dihydroxy-5-oxo-2*H*-furan-2-yl]-1,2-dihydroxyethyl] acetate

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

▸ PubChem

2.1.2 InChI

InChI=1S/C8H10O8/c1-3(10)16-8(14,2-9)6-4(11)5(12)7(13)15-6/h6,9,11-12,14H,2H2,1H3/t6-,8+/m0/s1

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

▸ PubChem

2.1.3 InChIKey

VYAIIIOLKRWRDE-POYBYMJQSA-N

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

▸ PubChem

2.1.4 SMILES

CC(=O)O[C@](CO)([C@@H]1C(=C(C(=O)O1)O)O)O

Computed by OEChem 2.3.0 (PubChem release 2024.12.12)

▸ PubChem

2.2 Molecular Formula

$C_8H_{10}O_8$

Computed by PubChem 2.1 (PubChem release 2019.06.18)

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2.3 Synonyms

2.3.1 Depositor-Supplied Synonyms

vitamin c acetate

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	234.16 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	-1.5	Computed by XLogP3 3.0 (PubChem release 2019.06.18)
Hydrogen Bond Donor Count	4	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	8	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)

Property Name	Property Value	Reference
Rotatable Bond Count	4	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	234.03756727 Da	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	234.03756727 Da	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	134 $Å^2$	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	16	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	359	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	2	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2016.09.28)

▸ PubChem

4 Related Records

4.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see the neighbor discontinuation help page for details), but these live search links provide equivalent functionality to the table that was previously shown here.

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4.2 Related Compounds

Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

▸ PubChem

4.3 Substances

4.3.1 Related Substances

Same Count	2

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4.3.2 Substances by Category

2 categories Download

Governmental Organizations (1)

PATENTSCOPE (WIPO)

PubChem SID: 390304701 External ID: VYAIIIOLKRWRDE-POYBYMJQSA-N

Journal Publishers (1)

Springer Nature

PubChem SID: 341712990 External ID: 16047684-868839690

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5 Literature

5.1 Consolidated References

PubChem

5.2 Springer Nature References

Springer Nature

5.3 Chemical Co-Occurrences in Literature

PubChem

5.4 Chemical-Gene Co-Occurrences in Literature

PubChem

5.5 Chemical-Disease Co-Occurrences in Literature

PubChem

5.6 Chemical-Organism Co-Occurrences in Literature

▸ PubChem

6 Patents

6.1 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=VYAIIIOLKRWRDE-POYBYMJQSA-N

▸ PATENTSCOPE (WIPO)

7 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. Springer Nature

   https://pubchem.ncbi.nlm.nih.gov/substance/341712990

2. PubChem

https://pubchem.ncbi.nlm.nih.gov

3. PATENTSCOPE (WIPO)

SID 390304701

https://pubchem.ncbi.nlm.nih.gov/substance/390304701

Cite Download

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